Automated System Software for the Standard Analysis Method (SAM)

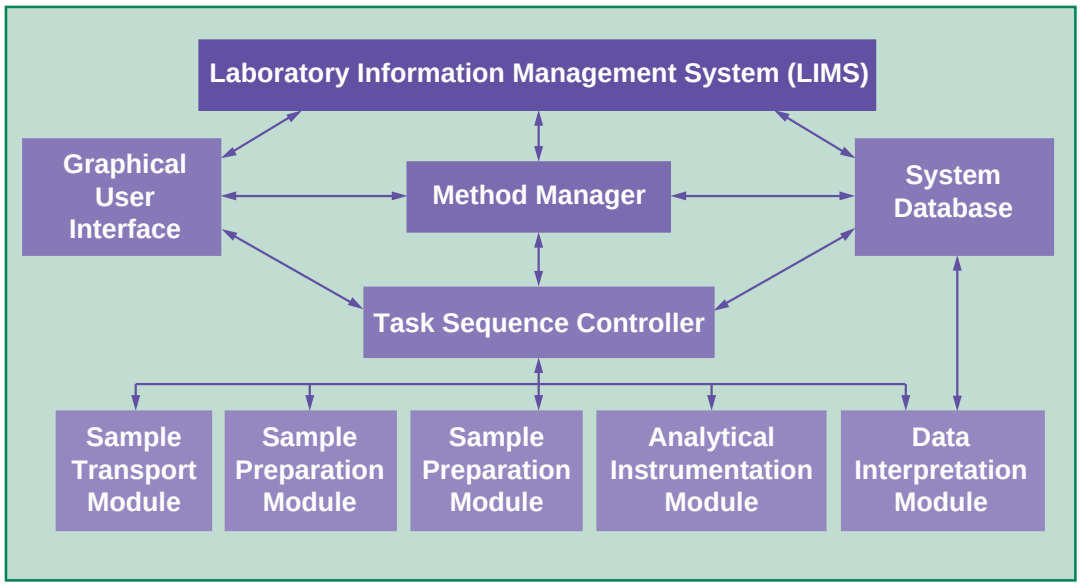

Figure 1. the CAA Software Architecture

Task Description

The goals of the system software development are to

- develop plug-and-play interface specifications for laboratory subsystems and laboratory software (control system, user interface, and database);
- establish a grammar for specifying analysis methods so they describe validated chemistry and are iandependent of any particular set of Standard Laboratory Module (SLMs™) that execute the method; and
- define an information model that enables the automated laboratory to archive sufficient data to satisfy regulatory and legal requirements.

To achieve these goals, the Contaminant Analysis Automation (CAA) team is developing software modules for a control system, user interface and database, and the specifications for the interfaces between these modules.

The SLMs™ are “plug and play” building blocks for the automated analytical chemistry laboratory. Each SLM™ can perform a subset of the operations required to implement automated chemical analyses, or SAMs. A SAM is programmed into the automated laboratory as a hierarchical script of chemical operations. The Task Sequence Controller (TSC) processes these scripts by expanding them into the primitive operations that can be performed by the individual SLMs™. It provides a single point of control over the SLMs™ in the laboratory. The database stores and provides access to all required information on the individual SLMs™, samples, and methods in order to enable system operation and ensure full QA / QC records. The figure shows these logical components of the automated laboratory and the relationships between them. The single arrow lines represent control connections, while the double arrow lines represent information exchange.

The key to modular chemistry is standardized interfaces between the components of the automated laboratory. All laboratory modules and subsystems must conform to a standard interface specification to ensure stylized interaction protocols. The SLM™ interface defines the interactions between the TSC and the SLMs™ attached to it. A supervisor-subsystem connection between the TSC and SLMs™ enforces a single point of control for on-line SLMs™ in the laboratory. The plug-and-play SLM™ interface requires standard mechanisms to permit the supervisor to determine the capabilities of the SLMs™ since the interface is independent of the operations an individual SLM™ performs. The TSC must also be able to coordinate physical interactions with an SLM™ (e.g., input and removal of samples and supplies), instruct the SLM™ to perform desired operations, and perform

various error-handling functions. The SLM™ interface consists of a set of commands and events, a process state behavior, an interaction protocol, and a capabilities data set.

The TSC is modeled after supervisory work cell controllers being developed and used for manufacturing environments. It perform tasks such as resource allocation and management and process monitoring. Traditionally, flow of material through the work cell is often driven by work cell capabilities and configuration. This means that production information is embodied in the work cell. Reconfiguration of this work cell requires reprogramming of the controller. Incorporation of new or improved capabilities into the work cell might require significant controller reprogramming. In contrast, the TSC is driven by what is termed the "smart item," where analysis information is associated with the item being operated on in the laboratory. This analysis information is entered into the controller as a method script programmed independently of any particular set of devices that may perform the chemical operations. Reconfiguration of the laboratory requires no change in controller or method scripts.

The database module is a distributed, C++ based, object-oriented database management system with internal client/server capabilities that permit data storage on different devices. An external user interface will enable the analytical chemist to browse through the database and select data for analysis. Database functionality is defined by the information needs of laboratory system setup and initialization, sample tracking, system maintenance, and data analysis. Sufficient data must be stored to legally support the analytical results.

The database design was based on the Analytical Data Interchange and Storage Standards constructs and the Consortium on Automated Analytical Laboratory Systems Modularity and Data Communications Standards. Modifications support CAA hardware components, provide easy waste tracking, and supply additional information necessary for the fully automated system.

Technology Needs

System software that completely tests all interface specifications is required to satisfy our goal of plug-and-play automated chemistry. In addition, a grammar for chemical method description is being developed.

Future system software development will focus on a method manager system that ensures that everything required for validated chemistry happens from a system standpoint. This module will ensure that calibrations, maintenance operations, control analyses, etc. are performed as required.

Accomplishments

- A standard interface specification for SLM™ communication and control interactions has been developed. A test bed of hardware and software modules is being implemented to test and enhance this specification.

- A TSC has been installed on the test bed, and integration with SLMs™ has been initiated. The TSC has begun integration with the HCI and database.

- A database communications interface with other software modules has been established. An initial database schema capable of storing and retrieving information has been implemented. This schema is being enhanced as test bed activities continue.

- A human/computer interface (HCI) with functionality for user access controls, process monitoring, and sample entry has been developed. This HCI has communication and control interfaces with both the TSC and the database. Testing of the HCI is in progress.

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